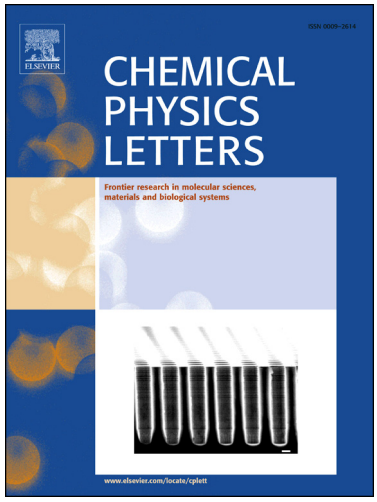

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Temperature induced transition from acceleration to deceleration of the diffusion of polymers by soft nanoparticles in their composite

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Abstract

It is well known that the presence of nanoparticles in polymer melt can dramatically influence the dynamics of the polymers. Here from a molecular dynamics simulation study, we find that such influences can be largely temperature dependent in a polymer/single chain nanoparticle composite. At high temperature, the translational diffusion of polymers can be accelerated due to large deformability of nanoparticle surface. While when temperature decreases, nanoparticle surface deformability decreases dramatically and therefore nanoparticles can impose large excess free energy barrier on polymer diffusion. As a consequence, the diffusion of polymers at low temperature can be largely decelerated.

Keywords: polymer/nanoparticle composite, polymer diffusion, soft nanoparticle, temperature effect

1. Introduction

Although incorporating nanaoparticles (NPs) into polymers can dramatically improve the properties of the material, [1, 2, 3, 4, 5] a thorough understanding of the influence of the loaded NPs on polymer dynamics in their composites is crucial for a better property design. Though this topic has recently been extensively investigated [6, 7, 8, 9, 10, 11, 12, 13], a full understanding of such influences, especially at different temperatures, is still

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